RISK-BASED CHEMICAL PROCESS ROUTE SELECTION CONSIDERING INHERENT ENVIRONMENTAL FRIENDLINESS

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Doctor of Philosophy

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April 2024

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Thesis submitted in partial fulfillment of the requirements for the degree

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DECLARATION

I declare that this is my own work and this thesis does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any other University or Institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text.

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The above candidate has carried out research for the PhD thesis under my supervision.

Name of Supervisor: Prof. (Ms.) Manisha Yasanthi Gunasekera

Signature of the Supervisor: Date: 01.04.2024.

ACKNOWLEDGEMENT

I would like to express my sincere gratitude to my supervisor, Professor Manisha Yasanthi Gunasekera, Department of Chemical and Process Engineering, University Moratuwa, for her exceptional mentorship and supervision throughout this research endeavour. Her profound expertise, scholarly guidance, and unwavering encouragement have been invaluable in completing this thesis. I am immensely grateful for her patience, availability, and continuous support, which have greatly enriched both my academic and personal growth.

I would also like to express my heartfelt gratitude to Professor P.G. Rathnasiri, former Head of the Department of Chemical and Process Engineering, University Moratuwa and Professor H. M. R. Premasiri, Department of Earth Resources Engineering, University Moratuwa for their insightful feedback, constructive criticism, and encouragement as the members in the progress review committee.

Furthermore, I am truly grateful to the academic and non-academic staff, and fellow research students of the Department of Chemical and Process Engineering, University of Moratuwa for supporting me whenever I needed it.

I would also like to express my sincere appreciation for the financial support provided by the University of Moratuwa Senate Research Grant. This research work was supported by the University of Moratuwa Senate Research Grant Number SRC/LT/2017/ 05.

I would like to extend my gratitude to my family for their love and support throughout my academic journey. I am also deeply appreciative of my friends, who have been there for me with uplifting conversations in challenging times. Finally, I want to express my gratitude to my loving husband Salika, for his constant patience, encouragement, and positive attitude throughout this entire journey.

Abstract

Chemical process route selection is one of the key decisions taken during the preliminary design stage of process plant development. A chemical process route is defined as the raw material(s) and the sequence of reaction step(s) that convert them to the desired product. In the past, the 'best' process route was selected solely considering economic factors. However, with the disastrous chemical plant accidents experienced in the past, attention has been drawn to select process routes considering other factors such as inherent environmental friendliness. Therefore, methodologies that assess chemical process routes considering environmental aspects are needed for the development of inherently environmentally friendly chemical process plants. The work presented in this thesis proposes a risk-based methodology to assess and rank chemical process routes considering inherent environmental friendliness using the data available during preliminary design stage of chemical process plant design and development. The environmental impacts that could occur due to chemical plant accidents such as accidental chemical releases, fires and explosions are considered when developing the methodology. In the proposed methodology, the chemical process routes are assessed in three approaches. They are fires and explosions, accidental chemical releases and all these three accidents in combination. Therefore, three risk indices are proposed namely, the Inherent Environmental Risk Index for Fires and Explosions (F&E-IERI), the Inherent Environmental Risk Index for accidental Chemical Releases (Chem-IERI), and the Inherent Environment Risk Index (Chem F&E-IERI). A lower risk index of a process route indicates a lower environmental risk and, thus the most inherently environmentally friendly route among the alternate process routes. The proposed methodology is applied in four potential process routes in acetone production. The results obtained show that the process route that has the lowest environmental risk due to fires and explosions in the chemical plant is the p-diisopropyl benzene oxidation process. The dehydrogenation of 2-propanol process route shows the lowest environmental risk due to accidental chemical release. The chemical route that has the lowest environmental risk due to all three major chemical plant accidents, fires, explosions, and chemical releases is the dehydrogenation of 2-propanol process.

Keywords: Environmental risk assessment, chemical process route selection, accidental chemical releases, fires and explosions, inherent safety

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LIST OF ABBREVIATIONS

Abbreviation	Description
$AcTL_j$	Minimum risk level of chemical *j* that is likely to be without appreciable risk of adverse non-cancer human health effects
aqlife	Aquatic life
BI	Burn injury impact
Chem-IERI	Inherent environmental risk index for accidental chemical release
CL_j	Concentrations (mol/m^3) in the atmosphere above which direct adverse effects on plants may occur according to present knowledge
F&E-IERI	Inherent Environmental Risk Index for Fires and Explosions
$f_{k,i,j}$	Frequency Index of chemical plant accident that results in environmental impact *k* due to chemical *j* in process equipment *i*
f_{ref}	Reference frequency of occurrence of fire and explosion event
GW	Global warming impact
i	Process equipment
$inhLC50_j$	Inhalation lethal concentration of chemical *j* that kills 50% of the test population of an animal species in 4 hours by inhalation, mol/m^3
$IR_{abs\,j}$	IR absorption strength of the chemical *j* in the interval of 500–1400 cm^{-1} , $cm^{-2}atm^{-1}$
j	Chemical in process equipment i
k	Environmental impact
$k_{OH(C_3H_6)}$	Rate constant for the reaction between the OH radical and propene
$k_{OH(j)}$	Rate constant for the reaction between the OH radical and substance *j*
LC_{50j}	Concentration of chemical *j* in water, which kills 50% of a test population of the most sensitive species over a 96 h period, mol/m^3
$LD_{50\,j}$	Lethal dose of chemical *j* that kills 50% of the test population (mg/kg)
LOC	Loss of containment
MM_j	Molecular mass of chemical *j*, g mol^{-1}
$M_{k,i,j}$	Magnitude of environmental impact *k*

n_{Cl}, n_{Br}	Number of Cl atoms per molecule, number of Br atoms per molecule
PECa,j	Predicted environmental concentration of the chemical *j* in the atmospheric compartment (mol/m^3)
PECa*(j)*	Predicted environmental concentration of substance *j* in ppbC in the atmospheric compartment when a quantity *Qj* is released
$PEC_{s\,j}$	Predicted environmental concentration of chemical *j* in soil compartment (mol/m^3)
$PEC_{w\,j}$	Predicted environmental concentration of chemical *j* in water compartment (mol/m^3)
Q_j	Quantity of the chemical *j* released into the atmosphere
g	acceleration due to gravity
RI_k	Risk index of environmental impact *k*
SD	Structural damage impact
$SM_{k,i,j}$	Scaled magnitude of environmental impact *k* of chemical *j* in process equipment *i*
s^n	Vulnerability score of n^{th} influencing factor
$TDI_{f,x,}$	Daily food intake of species x (m^3/day)
$TDI_{w,x}$	Daily fluid intake of species x (m^3/day)
terran	Terrestrial animal population
terrhab	Terrestrial habitants
veg	Vegetation
$Vgas_k$	Vulnerability score of the environmental element affected by environmental impact *k* due to accidental gas release
$Vliquid_k$	Vulnerability score of the environmental element affected by environmental impact *k* due to accidental liquid release
w_k	Weighting factor for environmental impact *k*
Wt_x	Weight of species x (kg)
τ_j	Atmospheric life (years) of chemical *j*

LIST OF APPENDICES